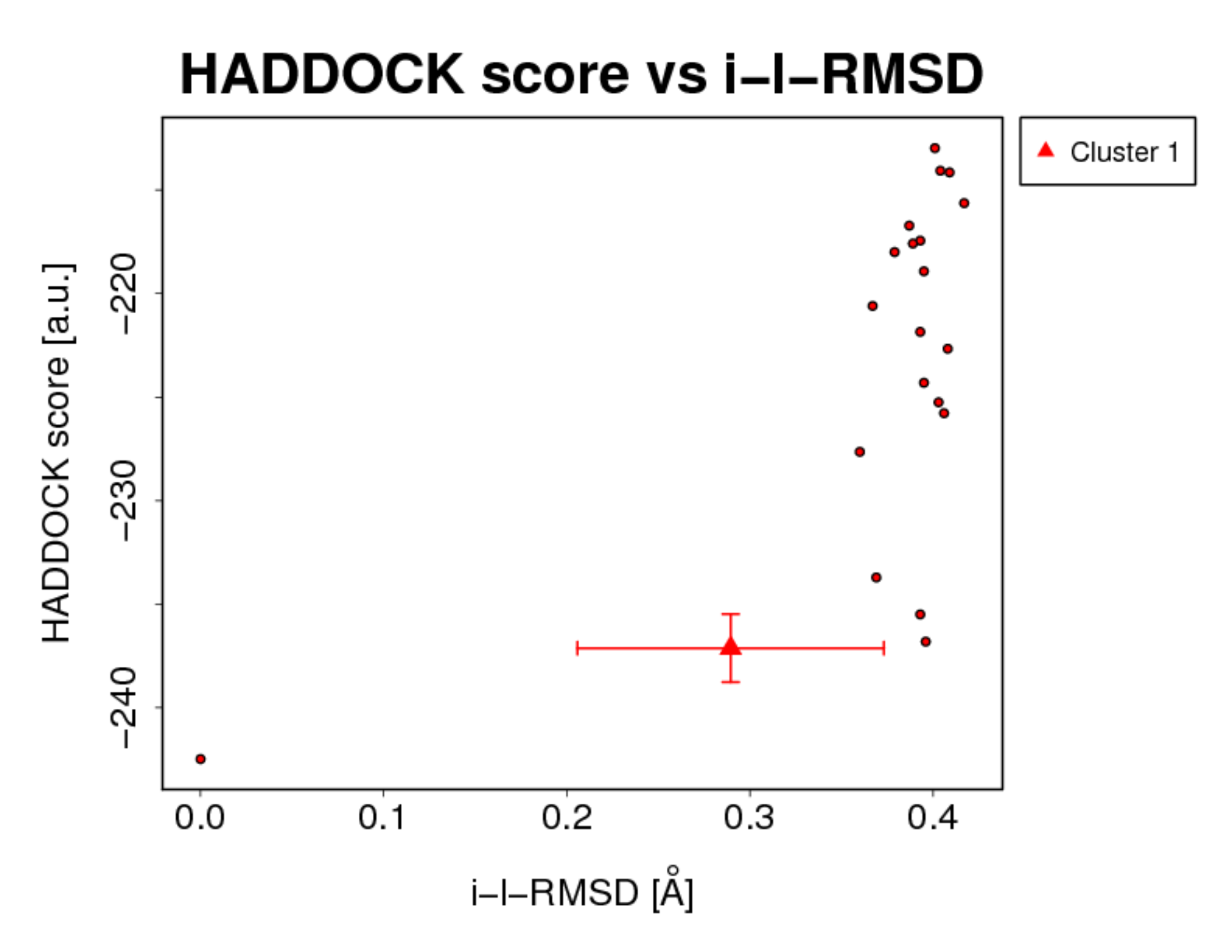
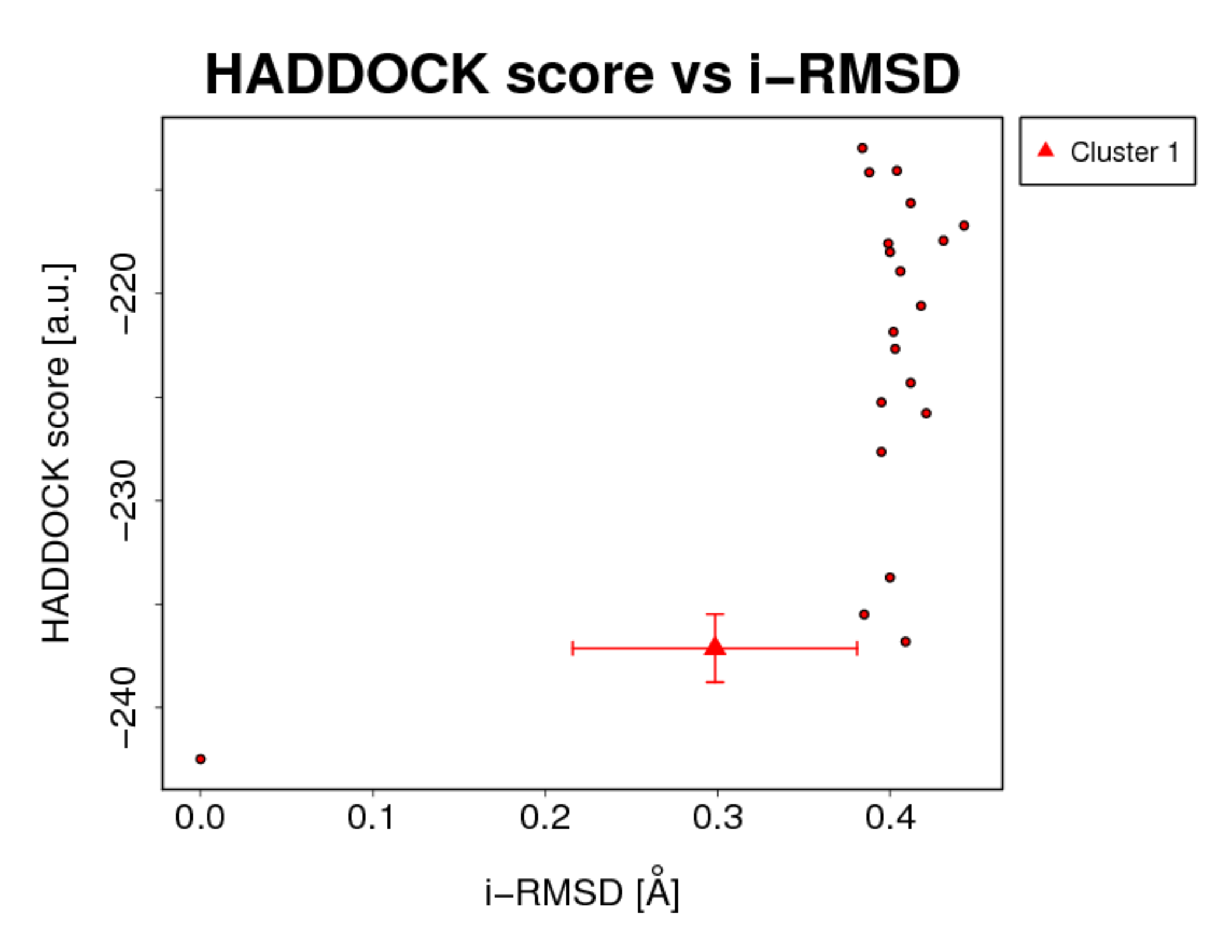
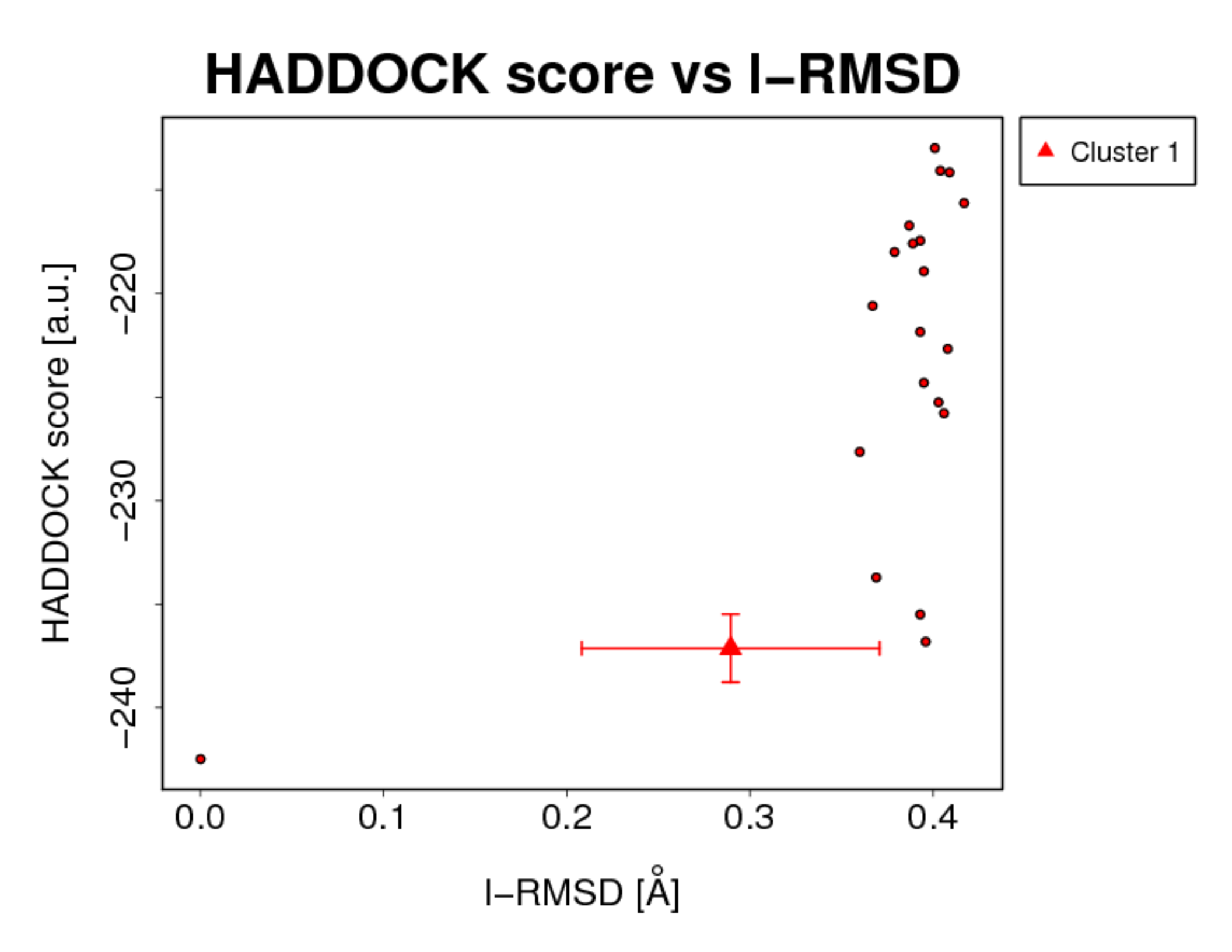
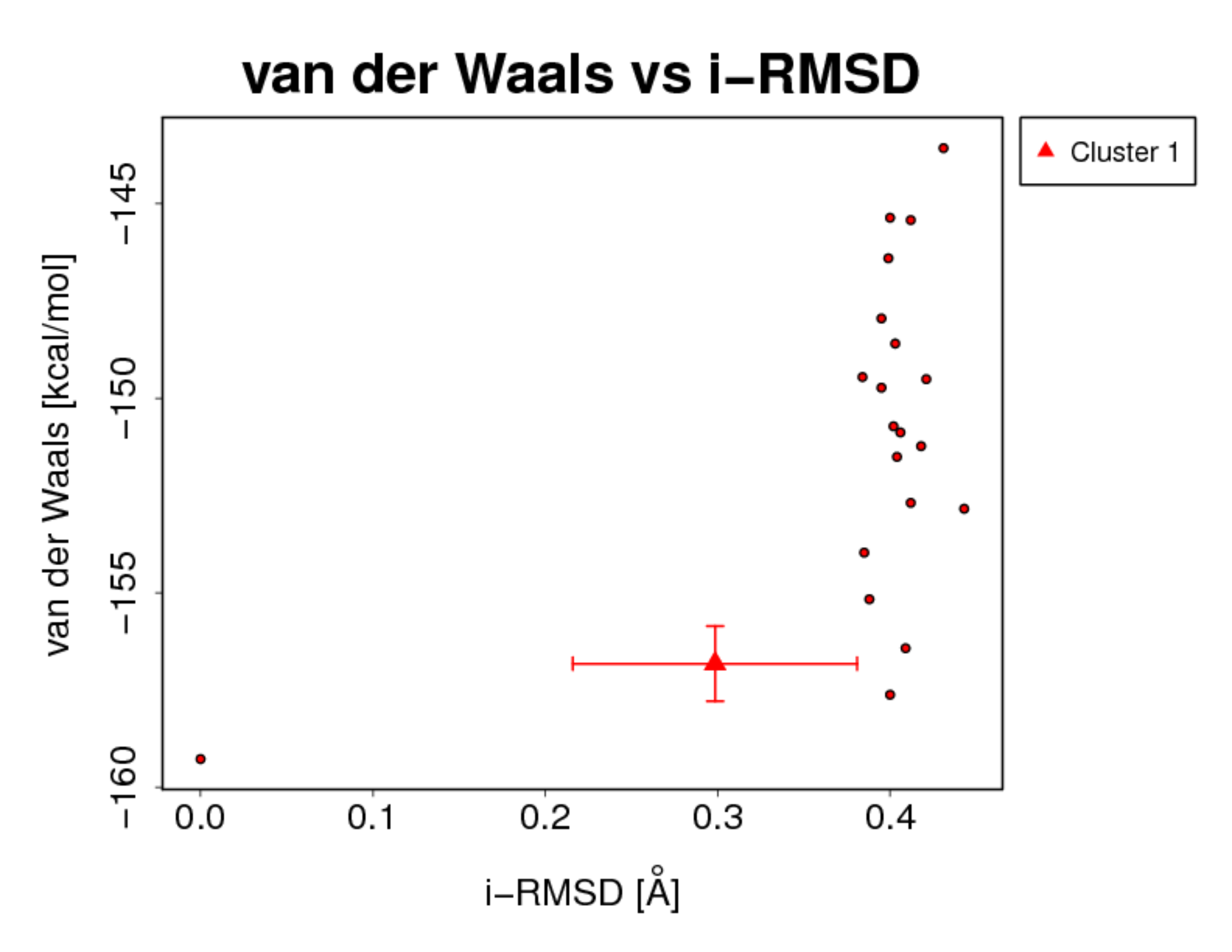
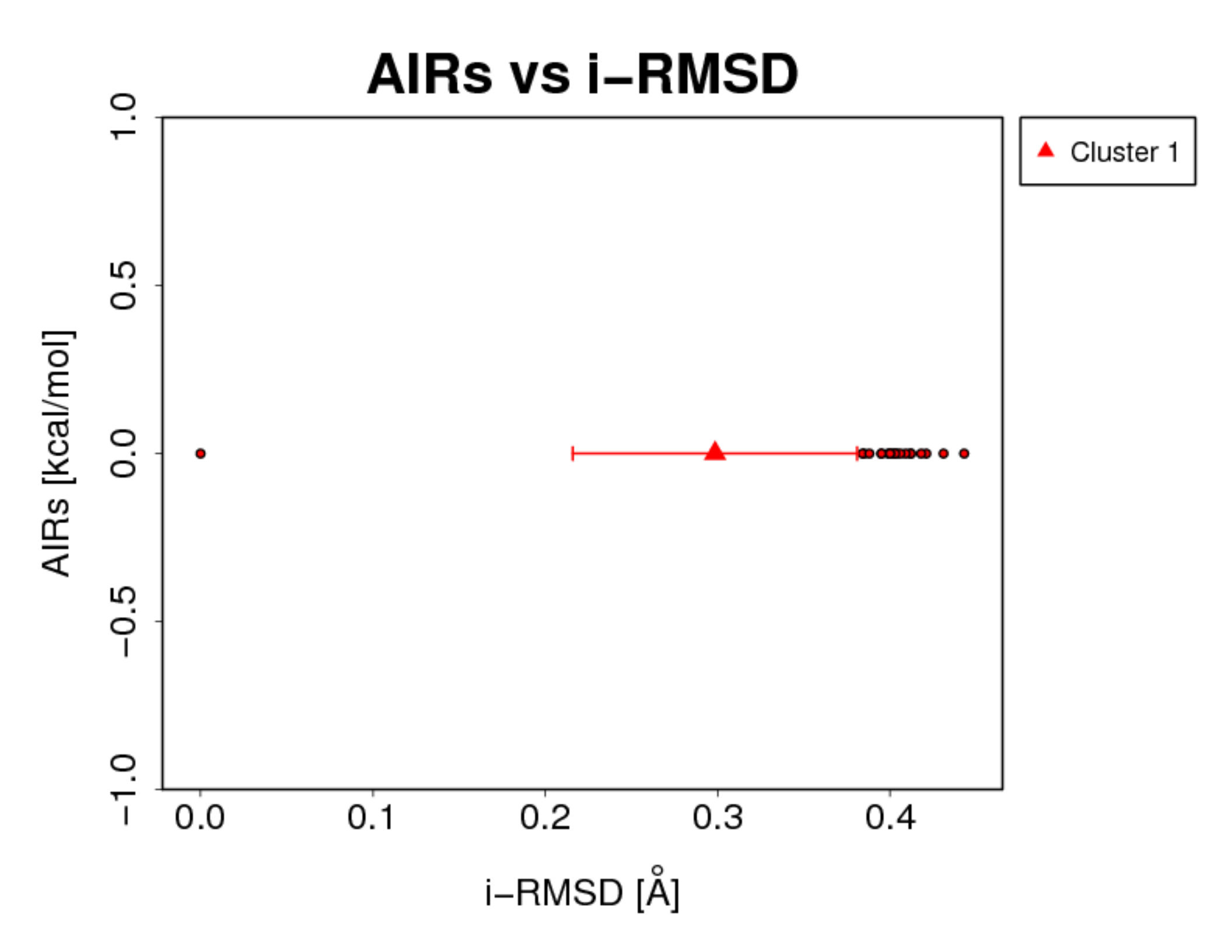
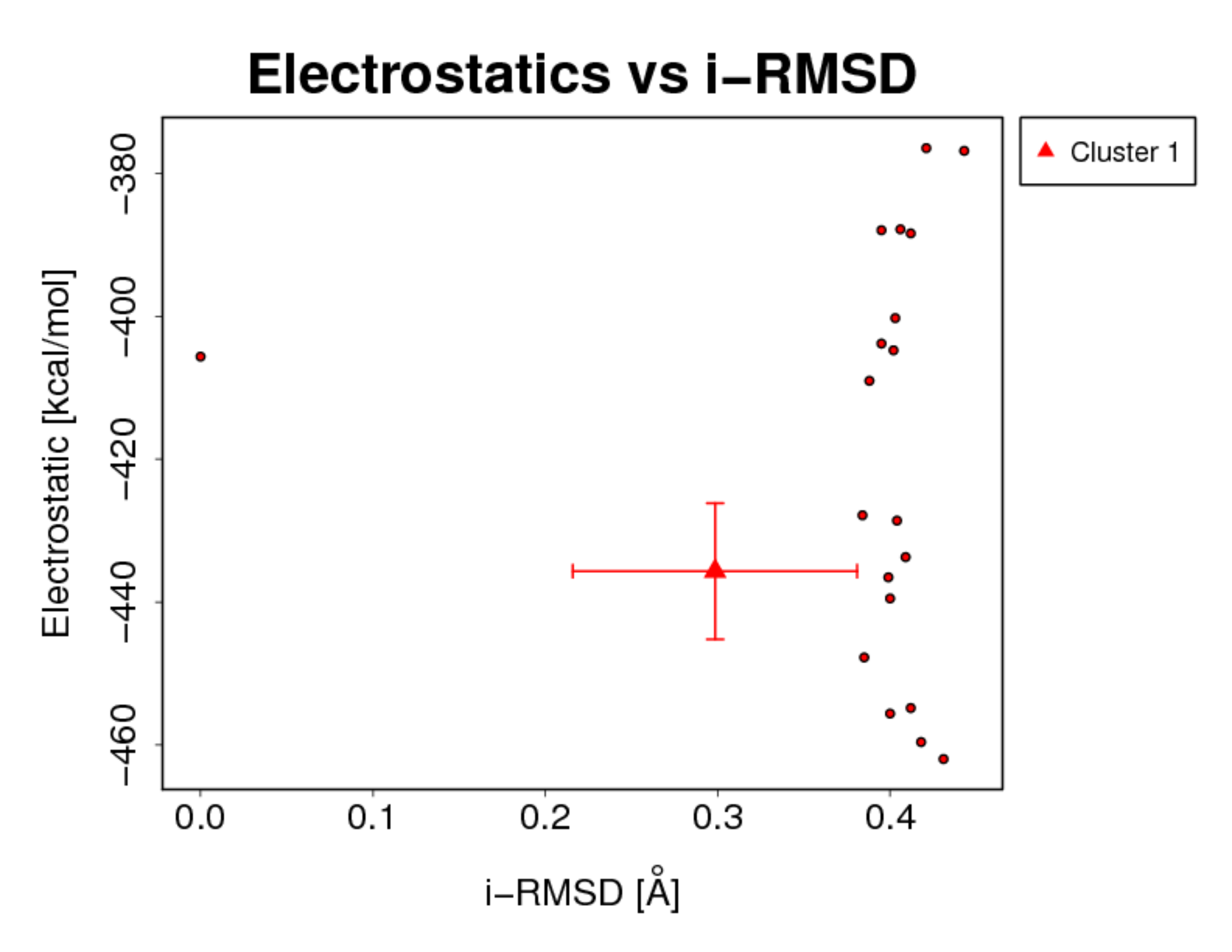

HADDOCK score vs i–l–RMSD
Cluster 1
HADDOCK score [a.u.]
−220
−230
−240
0.0
0.1
0.2
0.3
0.4
i–l–RMSD [Å]

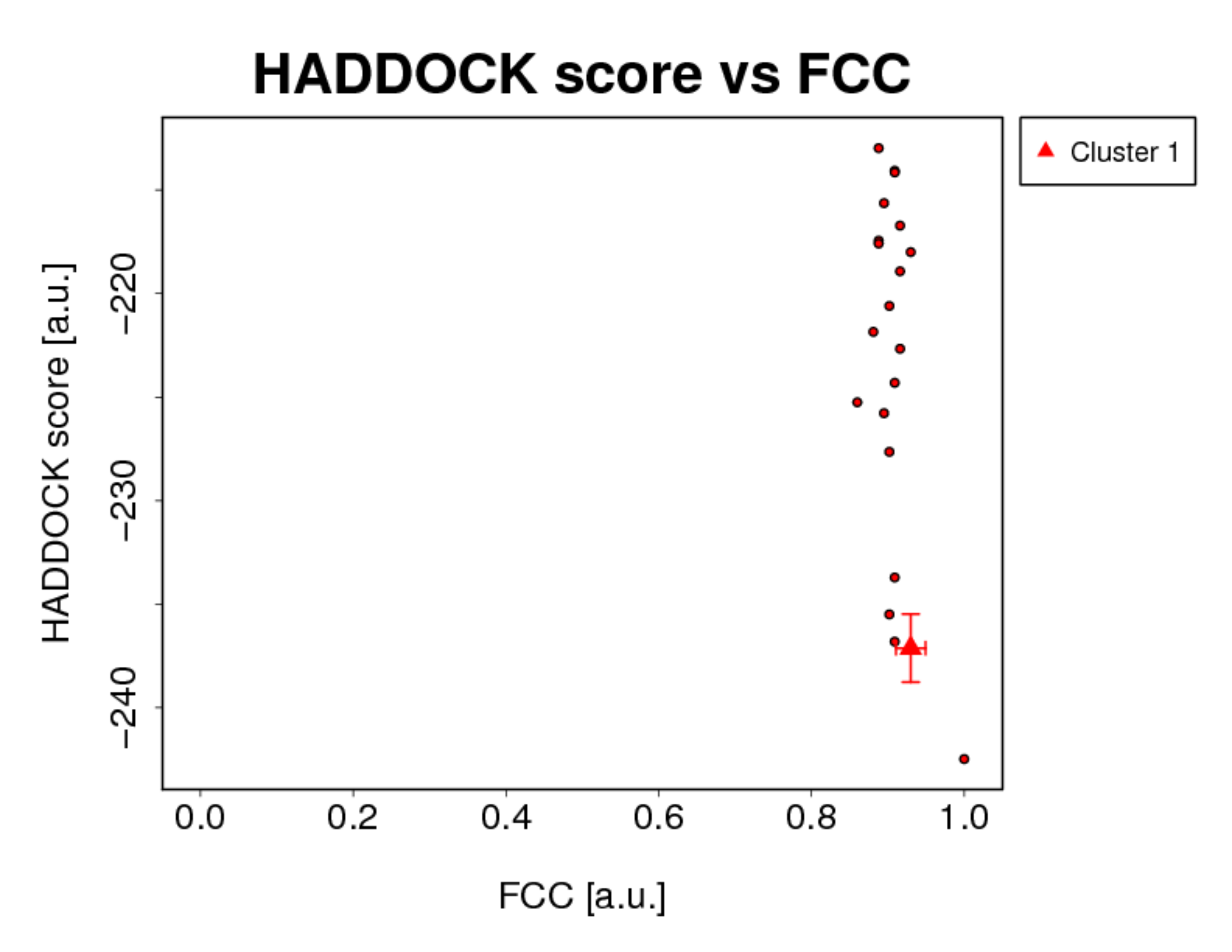

HADDOCK score vs i–RMSD
Cluster 1
HADDOCK score [a.u.]
−220
−230
−240
0.0
0.1
0.2
0.3
0.4
i–RMSD [Å]


HADDOCK score vs I–RMSD
Cluster 1
HADDOCK score [a.u.]
−220
−230
−240
0.0
0.1
0.2
0.3
0.4
I–RMSD [Å]


van der Waals vs i–RMSD
Cluster 1
van der Waals [kcal/mol]
−145
−150
−155
−160
0.0
0.1
0.2
0.3
0.4
i–RMSD [Å]


AIRs vs i–RMSD
AIRs [kcal/mol]
1.0
0.5
0.0
−0.5
−1.0
0.0
0.1
0.2
0.3
0.4
i–RMSD [Å]
Cluster 1


Electrostatics vs i–RMSD
Cluster 1
Electrostatic [kcal/mol]
−380
−400
−420
−440
−460
0.0
0.1
0.2
0.3
0.4
i–RMSD [Å]


HADDOCK score vs FCC
Cluster 1
HADDOCK score [a.u.]
−220
−230
−240
0.0
0.2
0.4
0.6
0.8
1.0
FCC [a.u.]